

TITLE: THERMOLYSIS OF DUVATRIENE-1,3-DIOLS

AUTHORS: T. Katz\*, R. D. Kinser, W. N. Einolf, and R. Bassfield

AFFILIATION: Philip Morris USA, Research Center, P.O. Box 26583,  
Richmond, VA 23261

ABSTRACT: Thermolysis at 250°C of the well-known tobacco diterpenes,  $\alpha$ - and  $\beta$ -4,8,13-duvatriene-1,3-diol is reported. The major products isolated from the decomposition mixtures are 5-isopropyl-8,12-dimethyl-3E,8E,12E,14-pentadecatetraen-2-one (I) and 3,7,13-trimethyl-10-isopropyl-2,6,11,13-tetradecatetraen-1-al (II). Previously we isolated (I) from cigarette smoke condensate and (II) by acid catalyzed ring-opening of the duvatriene-1,3-diols. The methods used to isolate and identify the precursor duvatriene-1,3-diols and their thermolysis products will be discussed. The duvatriene-1,3-diols were isolated from cuticular waxes that were removed from the surface of green tobacco leaves or tobacco flowering heads by non-polar solvents. The diols were separated from the waxes by methanol extraction or silica gel column chromatography. Reverse phase or normal phase HPLC was used to separate the  $\alpha$ -diol from the  $\beta$ -diol. Next, each diastereomeric diol was further purified by recrystallization; the physical properties of the recrystallized diols will be reported. The thermolysis products, (I) and (II), were isolated and their structures confirmed by GC, GC/MS and  $^1\text{H}$  NMR analyses. These results and a proposed mechanism for the formation of (I) and (II) will be discussed.

1000816891